Pfizer: NMR to ADF

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Pfizer Data: Scientific Data Cloud (SDC)

Capture

Lab Instruments & Software

Manufacturing Equipment

Data automatically swept into the cloud

Use

Lab IT Systems

Mobile Devices

Reports

Data is made available to systems and reports

IDF Scientific Data Cloud

Predict

Provides data need to build/run models

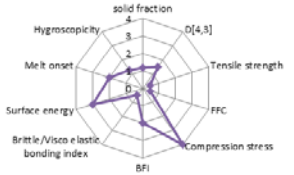
Predicted output from models is stored

Computational Models

Hosting Platforms

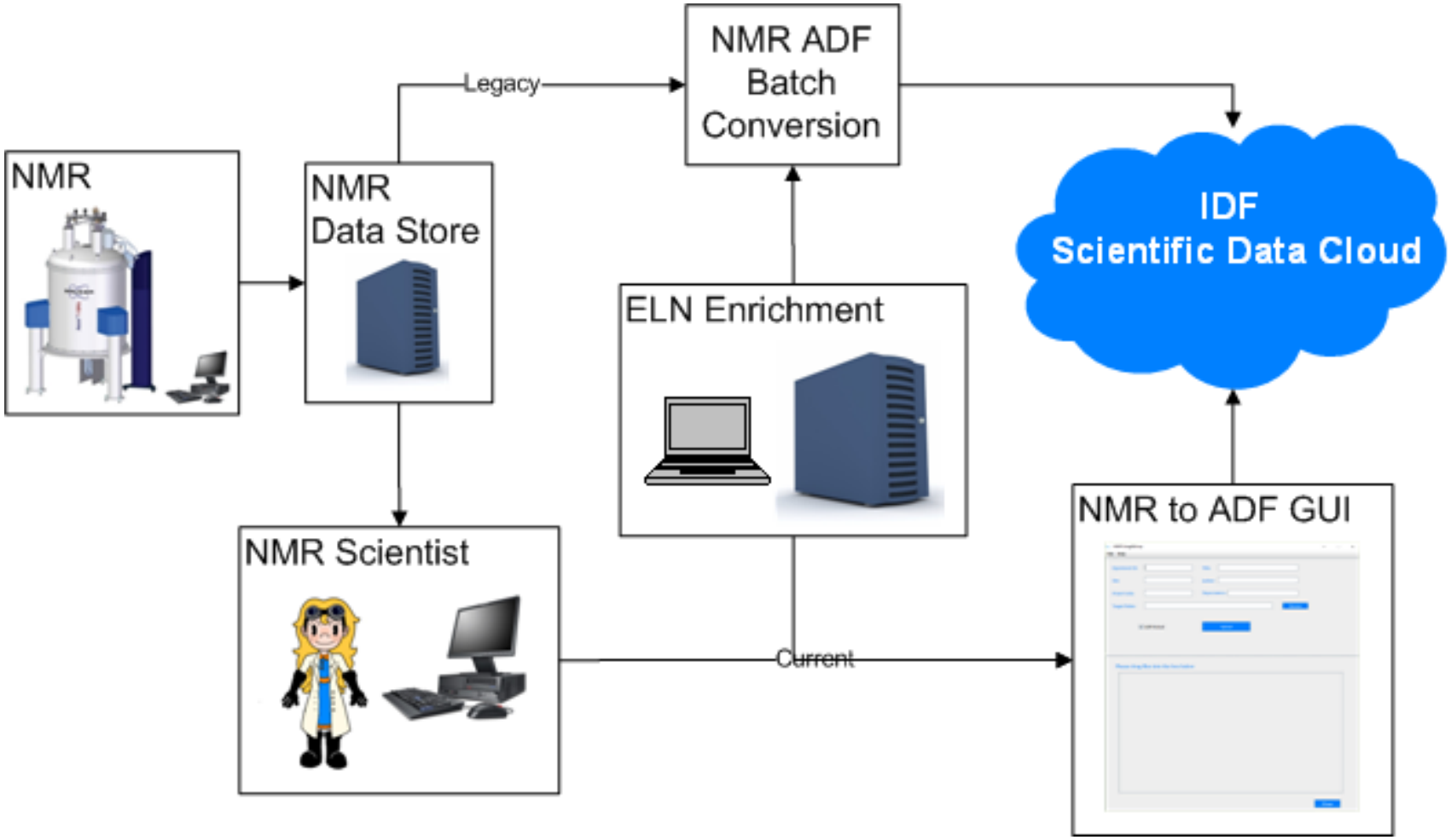
Reuse

Visualization tools are configured to pull data from the cloud



Data Visualization

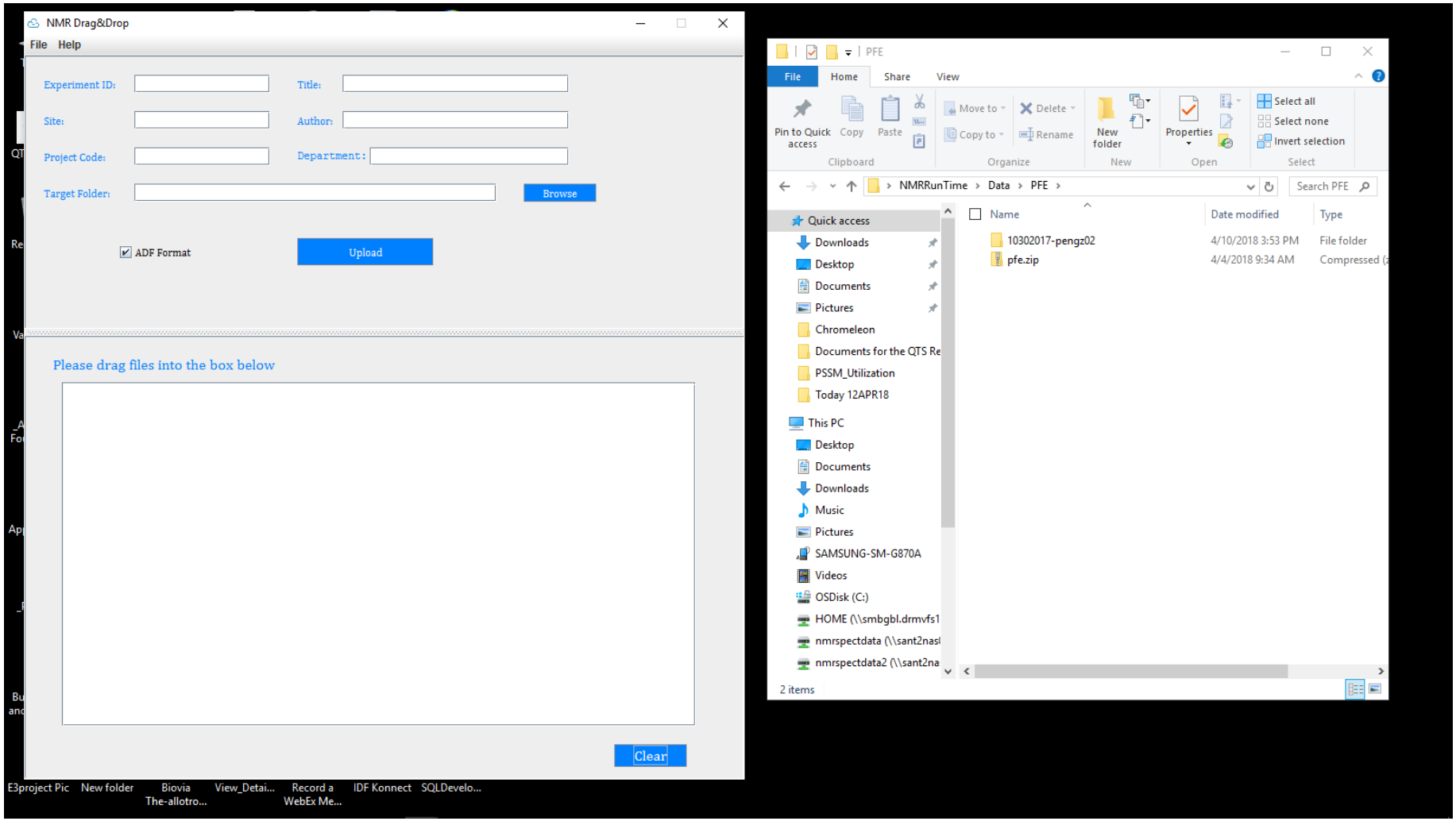
Pfizer: NMR to ADF Process Flow



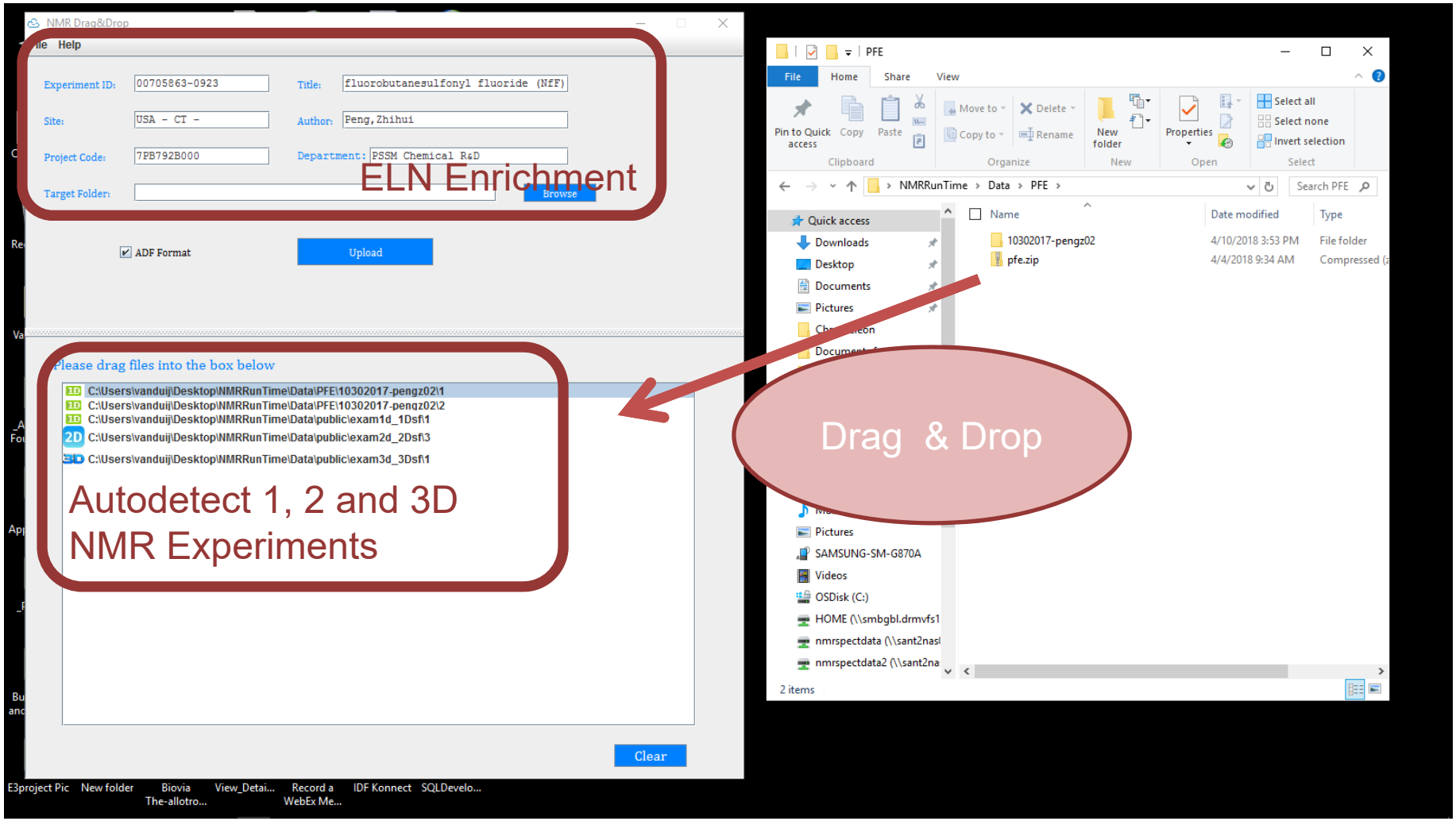
Enhancements to the Boehringer NMR Converter

- Transformed the user interface from a command line into a Graphic User Interface (GUI)
  - Encourages user adoption
  - Batch processing version is also available
- Uses current released versions of the Allotrope API's
- Extended to include 3D NMR data
- Added "Peak Table" to the Data Cube
- Creates a "Companion" JSON file to facilitate searching in the Pfizer SDC
- Added "important" meta data (including that from Pfizer's ELN) to the Data Description as literals
  - Does not use BFO/ADM

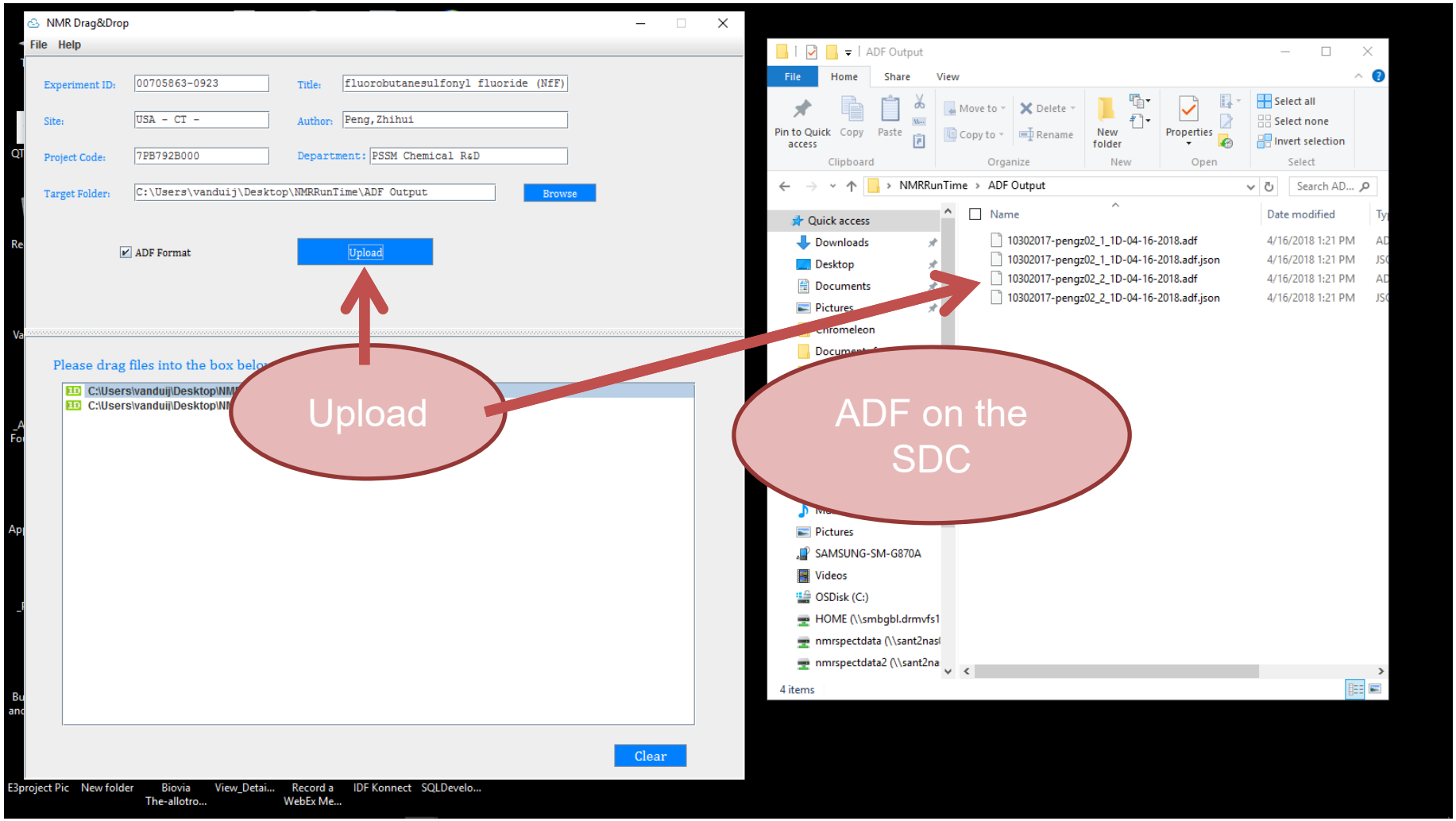
NMR to ADF Functionality (Converter GUI)



NMR to ADF Functionality



NMR to ADF Functionality



Companion File (JSON)

ELN Enriched Metadata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NMR Literal Metadata

ADF Explorer